Exploring the impact of ripples and electric fields on graphene's catalytic activity: a Density Functional Theory study

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Abstract:

Hydrogen (H2) is an important energy vector that can be used in fuel cells to produce carbon-free energy or as a clean fuel. In fuel cells, the dissociated H atoms react with oxygen (O2) to produce energy and water. However, the H2 dissociation reaction is an energy-expensive process and requires the usage of precious metals such as Platinum (Pt). These noble metals are expensive and are present in limited quantities. Therefore, alternative solutions need to be found to facilitate H2 dissociation.

Previous studies have shown that introducing ripples into the structure of graphene can help with increasing its activity as a catalyst and decreasing the energy barrier for H2 dissociation [1], [2]. Ripples can occur intrinsically in graphene and other 2D materials due to thermal fluctuations or they can be induced by applying a strain. Other studies [3], have explored the effect of the potential energy field of a material on the catalytic activity of graphene. In this work, first-principle density functional theory (DFT) is used to study the effect of the ripple and electric field on the graphene-H2 system and how they affect the energy barrier. The stability of the system and the energy barriers are obtained for different ripple heights and electric field magnitudes to fine-tune the best conditions for hydrogen dissociation.

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References

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